Machine Learning - Lecture 11: VC dimension

Chris Thornton

November 9, 2011

Decision-tree learning is typical of machine learning in its approach to model development.

Each time a split is introduced, the model is made a bit more detailed.

More training cases covered.

The model is said to be **incrementally refined** using the data as a source of reference.

Unfortunately, this approach produces problems if there are errors in the data (which there usually are).

▲日▼▲□▼▲□▼▲□▼ □ ののの

In this case there is the danger of reaching a point where refinements are simply 'learning the errors'.

This is known as **over-training** or **over-fitting**.

Fortunately, it is possible to detect over-fitting.

As model refinement continues we expect to see an improvement in performance on both seen and unseen data.

If the data contains some errors, there will come a point where refinements are simply modeling errors.

At this point, we should see deteriorating generalization, even while performance on seens continues to improve.

It is with this problem that cross-validation comes into its own.

We can use cross-validation methods to *detect* the point at which refinements appear to be producing the effect of over-fitting.

The idea is to terminate learning as soon as we go past the point where performance on unseen examples starts to deteriorate.

Unfortunately, in some situations, we see quite significant variations in generalization performance *prior* to any over-fitting.

Spotting the critical moment can be quite challenging.

More strongly biased methods are more limited in terms of the patterns they can represent.

So another way of making sure we don't end up 'training on noise' is to use a method whose bias effectively rules such patterns out.

In practice, this may be hard to achieve if we don't know what the errors are.

However, the general rule applies.

More strongly biased methods are more limited in terms of the patterns they can represent.

So another way of making sure we don't end up 'training on noise' is to use a method whose bias effectively rules such patterns out.

In practice, this may be hard to achieve if we don't know what the errors are.

However, the general rule applies.

• A stronger bias implies less vulnerability to over-fitting.

More strongly biased methods are more limited in terms of the patterns they can represent.

So another way of making sure we don't end up 'training on noise' is to use a method whose bias effectively rules such patterns out.

In practice, this may be hard to achieve if we don't know what the errors are.

However, the general rule applies.

- A stronger bias implies less vulnerability to over-fitting.
- A weaker bias implies more vulnerability.

More strongly biased methods are more limited in terms of the patterns they can represent.

So another way of making sure we don't end up 'training on noise' is to use a method whose bias effectively rules such patterns out.

In practice, this may be hard to achieve if we don't know what the errors are.

However, the general rule applies.

- A stronger bias implies less vulnerability to over-fitting.
- A weaker bias implies more vulnerability.

We want to achieve the strongest bias possible, but in a way that still allows significant patterns to be identified and represented.

VC definition

VC dimension is a formal measure of bias which has played an important role in mathematical work on learnability.

The VC dimension of a representation system is defined to be

◆□▶ ◆□▶ ◆三▶ ◆三▶ 三回 ● のへで

VC definition

VC dimension is a formal measure of bias which has played an important role in mathematical work on learnability.

The VC dimension of a representation system is defined to be

the maximum number of datapoints that can be separated (i.e., grouped) in *all* possible ways.

VC dimension is a formal measure of bias which has played an important role in mathematical work on learnability.

The VC dimension of a representation system is defined to be

the maximum number of datapoints that can be separated (i.e., grouped) in *all* possible ways.

Another way of saying this is to describe it as the the most datapoints that can be 'shattered' by the representation.

More powerful representations are able to shatter larger sets of datapoints. These have higher VC dimension.

Less powerful representations can only shatter smaller sets of datapoints.

These then have lower VC dimension.



4 datapoints cannot





◆□▶ ◆□▶ ◆三▶ ◆三▶ 三回 ● のへで

Model based on single linear division

VC dimension = 3

VC dimension seems to focus on a particularly demanding representation task, i.e., representing all possible ways of grouping datapoints.

From the intuitive point of view, this makes it less than ideal as a general measure of bias strength.

We could have a system with very low VC dimension that is actually quite weakly biased. This would happen, for example, if the system was able to *almost* shatter large datasets, while only being able to *fully* shatter very small ones.

VC dimension is useful in formal analysis of learnability, however.

This is because VC dimension provides an *upper bound* on generalization error.

The mathematics of this are quite complex.

The basic idea is that reducing VC dimension has the effect of eliminating potential generalization errors.

So if we have some notion of how many generalization errors are possible, VC dimension gives an indication of how many could be made in any given context.

The subfield of **Computational Learning Theory** is concerned with deriving VC-dimension bounds in different training scenarios.

Summary

With incremental model refinement we have the risk of 'training on noise', i.e,. over-fitting.

- With incremental model refinement we have the risk of 'training on noise', i.e,. over-fitting.
- A system that is over-fitting will tend to show deteriorating generalization.

◆□▶ ◆□▶ ◆三▶ ◆三▶ - 三 - のへぐ

- With incremental model refinement we have the risk of 'training on noise', i.e,. over-fitting.
- A system that is over-fitting will tend to show deteriorating generalization.
- Can address the problem through cross-validation strategies which aim to identify the point at which generalization starts to deteriorate.

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

- With incremental model refinement we have the risk of 'training on noise', i.e,. over-fitting.
- A system that is over-fitting will tend to show deteriorating generalization.
- Can address the problem through cross-validation strategies which aim to identify the point at which generalization starts to deteriorate.

▲日▼▲□▼▲□▼▲□▼ □ ののの

• Can also address the problem through strenghthening bias.

- With incremental model refinement we have the risk of 'training on noise', i.e,. over-fitting.
- A system that is over-fitting will tend to show deteriorating generalization.
- Can address the problem through cross-validation strategies which aim to identify the point at which generalization starts to deteriorate.
- Can also address the problem through strenghthening bias.
- VC dimension is a formal measure of bias that has been very useful in formal learning theory.

- With incremental model refinement we have the risk of 'training on noise', i.e,. over-fitting.
- A system that is over-fitting will tend to show deteriorating generalization.
- Can address the problem through cross-validation strategies which aim to identify the point at which generalization starts to deteriorate.
- Can also address the problem through strenghthening bias.
- VC dimension is a formal measure of bias that has been very useful in formal learning theory.

Questions

How does the problem of over-fitting arise in the case of k-means clustering?

- How does the problem of over-fitting arise in the case of k-means clustering?
- How does the problem of over-fitting relate to the problem of lookup tables?

◆□▶ ◆□▶ ◆三▶ ◆三▶ - 三 - のへぐ

- How does the problem of over-fitting arise in the case of k-means clustering?
- How does the problem of over-fitting relate to the problem of lookup tables?
- Consider a representational framework based on centroids in a 2d space. What is the VC dimension?

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

- How does the problem of over-fitting arise in the case of k-means clustering?
- How does the problem of over-fitting relate to the problem of lookup tables?
- Consider a representational framework based on centroids in a 2d space. What is the VC dimension?

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @